

Influence of scattering processes on electron quantum states in nanowires

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Abstract In the framework of quantum perturbation theory the self-consistent method of calculation of electron scattering rates in nanowires with the one-dimensional electron gas in the quantum limit is worked out. The developed method allows both the collisional broadening and the quantum correlations between scattering events to be taken into account. It is an alternative *per se* to the Fock approximation for the self-energy approach based on Green's function formalism. However this approach is free of mathematical difficulties typical to the Fock approximation. Moreover, the developed method is simpler than the Fock approximation from the computational point of view. Using the approximation of stable one-particle quantum states it is proved that the electron scattering processes determine the dependence of electron energy versus its wave vector.

Keywords Nanowire · Electron scattering · Electron quantum states · Collisional broadening · Quantum correlations

Introduction

Presently the interest to nanoscale electronics increases dramatically. At that the great attention is paid to structures containing the one-dimensional electron gas such as nanowires and nanotubes. However, to develop devices using structures like that [1, 2] it is necessary to

have the profound description of the kinetic processes determining the electrophysics of the structures with one-dimensional electron gas. The description of the kinetic processes calls forth the need of developing the theory of electron scattering in nanoscale structures with one-dimensional electron gas. For example, in Ref. [3] the model of electron transport in the armchair single-wall carbon nanotubes has been developed. This model is based on the numerical solution of the Boltzmann equation. It allows the current-voltage characteristics to be calculated with high concordance with results of experiments. While creating this model some questions concerning the features of electron scattering in cylindrical symmetry quantum systems have been cleared up. At the same time while developing a similar model of electron transport in nanowires, taking into account the high-order quantum effects (the collisional broadening and the quantum correlations between scattering events) (see, for example, Refs. [4–8]), we have met a problem. It is turned out that some obtained results are in contradiction to the fundamental physical principles. This paper is devoted to description of the essence of the problem and the way to solve it.

Theory

It is known when the quasi-classical one-particle (Hartree-Fock) approximation [9–11] is valid to describe the electron transport, the state of one-dimensional electron gas is determined by the Boltzmann transport equation [3, 11–14]

$$\left(\frac{d}{dt} + \hat{I}\right)f(x, k, t) = 0, \quad (1)$$

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where \hat{T} is the collisional operator, f is the electron distribution function, x is the coordinate along nanowire, k is the electron wave vector, t is the time.

If the electric field is absent the electron gas is in the equilibrium state. Consequently, electron energy distribution function is the Fermi-Dirac one, i.e. the following equation is valid

$$\hat{T}f(k) = \hat{T}f_F(k) = 0, \quad (2)$$

where f_F is the Fermi-Dirac distribution function.

If the scattering rates in one-dimensional electron gas are calculated according to the Fermi golden rule [9, 15] taking into account nonparabolicity [12, 13] as well as neglecting the latter it is easy to make sure that Eq. (2) is valid. However, when the scattering rates are calculated taking into account high-order quantum effects such as the collisional broadening [4–8] and the quantum correlations between scattering events [4], Eq. (2) is no longer valid. Thus in this case we should split Eq. (2) in

$$\hat{T}f(k) = 0, \quad (3)$$

$$\hat{T}f_F(k) \neq 0. \quad (4)$$

It results in $f \neq f_F$.

Thus, the contradiction takes place. From one hand, electrons should be distributed according to the Fermi-Dirac law [9–11, 14] without regard to presence or absence of scattering. It is called forth by the antisymmetry of the wave function of electron gas at the considered approximation. From other hand, the distribution function should be in accord with Boltzmann equation. Nevertheless, it is impossible according to Eqs. (3) and (4).

This contradiction can be easily explained taking into account that as a matter of fact the Boltzmann transport equation is nothing but approximation of the Liouville quantum equation [9, 16] at smooth and slowly varying potential (i) and using the approximation of stable one-particle quantum states [11] for all calculated physical quantities (ii). When one calculates a physical quantity beyond these approximations and substitutes it into the Boltzmann equation the obtained results contradict the fundamental physical principles. Thus, the considering contradiction (see Eqs. (3) and (4)) is caused by violation of the approximations that the electron quantum states are stable or/and one-particle while calculating the electron

scattering rates taking into account the high-order quantum effects [4–8].

Generally speaking, there are quantum mechanical methods to solve such problems [9–11, 16]. However, from the mathematical and computational point of view these methods are more difficult than approaches based on the numerical solution of the Boltzmann equation [3, 12, 13]. In this connection we consider the electron transport in the framework of approximation of the Boltzmann transport equation. To avoid violation of the conditions mentioned above it is necessary to consider the electron transport like the transport of quasi-particles of electron gas. It is one of standard techniques of the quantum mechanics (see, for example, Ref. [9]). These techniques allow the mathematical form of equations to be preserved. In this case the dependence of quasi-particle energy versus its wave vector $E = E(k)$ is different from one for the case of free electrons [9].

To obtain the mentioned dependence one can use the canonic transformation method [9]. However we are finding the dependence $E = E(k)$ in the indirect way. Let us postulate Eq. (2) using the scattering rates derived taking into account the high-order quantum effects. To do it we use the results of Refs. [5–8]. In these studies the scattering rates in GaAs quantum wires have been calculated taking into consideration the collisional broadening of the initial electron quantum states (electron energy uncertainty). At that according to Refs. [4, 6, 7] the influence of the collisional broadening on the scattering matrix element is too small to take effect on the scattering rates. So, this influence can be neglected or be taken into consideration only in the first order approximation. Then it mainly takes effect on density of states.

To derive the high precision function $E = E(k)$ it is necessary to take into account the quantum correlations between scattering events. It can be done considering that the sequence of N scattering acts is terminated by $(N+1)$ one at $N \rightarrow +\infty$ instead of considering that the only scattering act is terminated by the next one. In this case according to Refs. [5–8] to take into account the quantum correlations between scattering events it is sufficient to consider the collisional broadening of the final electron quantum states as well as initial and final states identity at $k_{\text{initial}} = k_{\text{final}}$. In result, the equations for the self-consistent calculation of the function $E = E(k)$ for the one-dimensional electron gas in the electric quantum limit and thermodynamic equilibrium can be derived by

$$\begin{aligned} \frac{2\Delta E}{\hbar} = \sum_i \left\{ 2C_i^{\text{el}} \left[\left| M_i^{\text{e/f}}(k_0(\Delta E/2)) \right|^2 + \left| M_i^{\text{el/b}}(k_0(E + \Delta E/2)) \right|^2 \right] \rho(E, \Delta E)(1 - f_F(E)) + \right. \\ C_i^{\text{e}} \Theta(E - \hbar\omega_i) \left| M_i^{\text{e/(f+b)}}(k_0(E), k_0(E - \hbar\omega_i)) \right|^2 \rho(E - \hbar\omega_i, \Delta E)(1 - f_F(E - \hbar\omega_i)) + \\ C_i^{\text{a}} \Theta(E + \hbar\omega_i) \left| M_i^{\text{a/(f+b)}}(k_0(E), k_0(E + \hbar\omega_i)) \right|^2 \rho(E + \hbar\omega_i, \Delta E)(1 - f_F(E + \hbar\omega_i)) + \\ C_i^{\text{e}} \Theta(E + \hbar\omega_i) \left| M_i^{\text{e/(f+b)}}(k_0(E), k_0(E + \hbar\omega_i)) \right|^2 \rho(E, \Delta E)(1 - f_F(E)) + \\ \left. C_i^{\text{a}} \Theta(E - \hbar\omega_i) \left| M_i^{\text{a/(f+b)}}(k_0(E), k_0(E - \hbar\omega_i)) \right|^2 \rho(E, \Delta E)(1 - f_F(E)) \right\}, \end{aligned} \tag{5}$$

$$\rho(E) = \rho(E, \Delta E(E)) = \left| \frac{dE}{dk} \right|^{-1} = \int_0^\infty \rho_0(\xi) s(\xi, E, \Delta E(E)) d\xi, \tag{6}$$

$$k(E) = \int_0^E \rho(\xi) d\xi, \tag{7}$$

$$E(k) = k^{-1}(E). \tag{8}$$

Here \hbar is the Planck constant, ΔE is the collisional broadening factor [5–8], C is the normalization factor determined by means of the Fermi golden rule, M is the scattering matrix element, ω is the cyclic phonon frequency, Θ is the Heaviside function, s is the spectral function [6]. Index “el” corresponds to elastic scattering processes. Indexes “e” and “a” correspond to inelastic scattering processes. Index “e” means phonon emission, and index “a” means phonon absorption. Indexes “f” and “b” correspond to forward and backward scattering, respectively. The parameters of scattering mechanisms of the same class are marked with low index “i”. Low index “0” shows that it is necessary to use the standard dispersion relations for free electrons while calculating the corresponding physical quantity.

It should be noted that the use of the approximation $k_0(E)$ is valid for the most of dominant scattering mechanisms due to the fact that the dependence of scattering matrix elements versus k is smooth in the vicinity of $k=0$ (see, for example, Refs. [6–8]). The use of the exact function $k(E)$ makes calculation of $E = E(k)$ more complicated from mathematical and computational point of view due to need of solving of the integral equation instead of the transcendent one (5). The integral equation is obtained while substituting the right part of Eq. (7) to the right part of Eq. (5). It is called forth by the fact that function $\rho(E) = \rho(E, \Delta E(E))$ is the explicit function of E and ΔE (see, for example, Refs. [5–8]) whereas the function $\Delta E(E)$ is unknown *a priori*. The latter is determined by means of solution of Eq. (5). In result, the function ρ versus E is an implicit one, indeed. Just because of this

circumstance the integral equation takes place when the exact function $k(E)$ is used.

Also it should be noted that the Eq. (5) is written in the terms of the final quantum states instead of the initial ones [5–8]. Such a representation is made for the convenience of scattering rate calculations. Moreover, it should be outlined that the approximations of the electric quantum limit and thermodynamic equilibrium are considered to reduce the unhandiness of the equations. These approximations are not principle. For example, considering the non-equilibrium electron gas it should be taken into account that the population of the final quantum states is determined by non-equilibrium electron distribution function instead of the Fermi-Dirac one. Consequently, the number of terms in Eq. (5) increases nearly in two times. This number also increases if the exited states are taken into account due to the terms bearing relation to intersubband transitions [5].

The expressions for calculation of the rates of elastic W^{el} and inelastic $W^{\text{e/a}}$ electron scattering derived in the framework of the approximation of stable one-particle quantum states in the one-dimensional electron gas in the quantum limit and thermodynamic equilibrium are presented in the following explicit form:

$$W_i^{\text{el}}(E) = C_i^{\text{el}} \rho(E, \Delta E(E)) \left[\left| M_i^{\text{e/f}}(k_0(\Delta E(E)/2)) \right|^2 + \left| M_i^{\text{el/b}}(k_0(E + \Delta E(E)/2)) \right|^2 \right] (1 - f_F(E)), \tag{9}$$

$$W_i^{\text{e}}(E) = C_i^{\text{e}} \Theta(E - \hbar\omega_i) \left| M_i^{\text{e/(f+b)}}(k_0(E), k_0(E - \hbar\omega_i)) \right|^2 \times \rho(E - \hbar\omega_i, \Delta E(E - \hbar\omega_i))(1 - f_F(E - \hbar\omega_i)), \tag{10}$$

$$W_i^{\text{a}}(E) = C_i^{\text{a}} \Theta(E + \hbar\omega_i) \left| M_i^{\text{a/(f+b)}}(k_0(E), k_0(E + \hbar\omega_i)) \right|^2 \times \rho(E + \hbar\omega_i, \Delta E(E + \hbar\omega_i))(1 - f_F(E + \hbar\omega_i)). \tag{11}$$

It can be proved that $\widehat{I}f_F = 0$ if the collisional operator \widehat{I} is determined by Eqs. (9)–(11).

Results and discussion

Let us consider some results of application of the developed theory to calculate the dependence of $E(k)$ and the electron scattering rates in the electric quantum limit and thermodynamic equilibrium taking into account the nonparabolicity. Let us consider GaAs-in- Al_2O_3 quantum wires with a straight heterointerface and the cross-section of $10 \times 10 \text{ nm}^2$. In this case it is valid to use the approximation of infinite depth quantum well and to neglect the surface roughness scattering. It is assumed that doping of GaAs meets both the condition that at considered temperature $T = 300 \text{ K}$ the Fermi level is approximately 0.2 eV lower than the energy level of the ground quantum state and the condition that the ionized impurity scattering can be neglected. We are also neglecting the acoustic phonon scattering. Thus, the polar optical phonon scattering is the last dominant scattering mechanism (see Refs. [6–8]). Taking into account that the difference between the values of dielectric permittivity of GaAs and Al_2O_3 is small the surface polar optical phonon scattering can be neglected [15]. The localized phonon modes should be taken into consideration only [15]. Due to the electric quantum limit condition it is valid to consider the first phonon mode only, because others have a very small influence on the intrasubband electron scattering in the ground quantum state [5, 8, 15].

The results of calculation of the polar optical phonon scattering rates in GaAs-in- Al_2O_3 quantum wire are

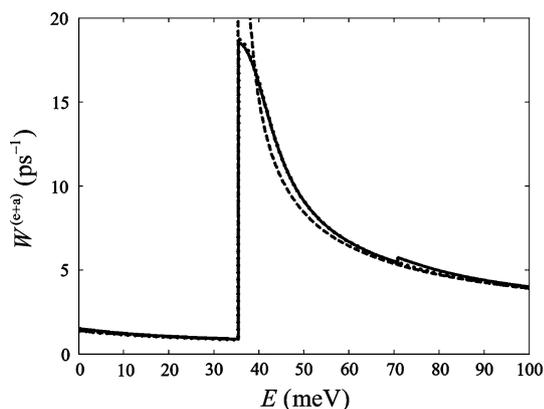


Fig. 1 Polar optical phonon scattering rates ($W^{e+ia} = W^e + W^a$). Solid curve: the results of self-consistent calculations (Eqs. (10), (11)). Dotted curve: the results obtained in the framework of theoretical model of Refs. [6, 8]. Dashed curve: the results obtained in the framework of the Fermi golden rule

presented in Fig. 1. They are obtained within the approximations discussed above. The results of Ref. [4] are shown in Fig. 2. Analyzing these figures one can conclude that the results obtained by using the developed method are in a reasonable agreement with the ones obtained by using the Fock approximation for the self-energy approach based on Green's function formalism. As it was noted in Ref. [8] some discrepancy between the results shown in Figs. 1 and 2 is called forth by considering the bulk phonons in Ref. [4] whereas we have considered the localized ones. Fig. 1 shows that taking into account the quantum correlations between scattering events causes the slight step increase of scattering rates at $E \geq 2\hbar\omega$. Almost the same feature takes place in Fig. 2.

To prove the validity of the developed model let us calculate the rate of electron scattering due to the polar optical phonons by using both our technique and the Fock approximation for the self-energy approach under the same conditions. The nonparabolicity and the Pauli principle are neglected to simplify the problem. Moreover, we take under consideration a hypothetical case when the quantum wire is infinitely thin. At that the electron-phonon coupling constants do not depend on the components of the electron and phonon wave vectors parallel to the wire [4]. Taking into account these assumptions the calculation of the self-energy under the Fock approximation can be reduced to the transcendent equation [4, 11]

$$\begin{aligned} \Sigma(\varepsilon) &= \Sigma_e(\varepsilon) + \Sigma_a(\varepsilon) \\ &= \frac{-i\sqrt{2m^*}}{4\hbar} \left(\frac{g_e^2}{\sqrt{\varepsilon - \hbar\omega - \Sigma(\varepsilon - \hbar\omega)}} \right. \\ &\quad \left. + \frac{g_a^2}{\sqrt{\varepsilon + \hbar\omega - \Sigma(\varepsilon + \hbar\omega)}} \right), \end{aligned} \quad (12)$$

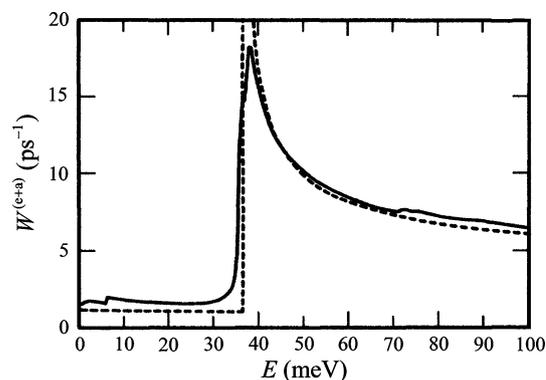


Fig. 2 Polar optical phonon scattering rates taken from Ref. [4]. Solid curve: the results obtained in the framework of the Fock approximation. Dashed curve: the results obtained in the framework of the Fermi golden rule

where Σ is the electron-phonon self-energy, m^* is the electron effective mass, $g_{e/a}^2$ is the electron-phonon coupling constant corresponding to emission/absorption process.

The mean relaxation rate of the one-particle excited state due to electron-phonon interaction can be formulated as [4, 11]

$$W_{\Sigma}(E) = W_{\Sigma}^e(E) + W_{\Sigma}^a(E) = -\frac{2}{\hbar} \text{Im}(\bar{\Sigma}_e(E) + \bar{\Sigma}_a(E)) = -\frac{2}{\hbar} \text{Im}(\bar{\Sigma}(E)) = -\frac{2}{\hbar} \text{Im} \left(\int_{-\infty}^{+\infty} \Sigma(\varepsilon) S(\varepsilon, E) d\varepsilon \right), \tag{13}$$

$$S(\varepsilon, E) = \frac{-2\text{Im}(\Sigma(\varepsilon))}{[\varepsilon - E - \text{Re}(\Sigma(\varepsilon))]^2 + [\text{Im}(\Sigma(\varepsilon))]^2} \times \left(\int_{-\infty}^{+\infty} \frac{-2\text{Im}(\Sigma(\varepsilon))}{[\varepsilon - E - \text{Re}(\Sigma(\varepsilon))]^2 + [\text{Im}(\Sigma(\varepsilon))]^2} d\varepsilon \right)^{-1}, \tag{14}$$

$$E = \frac{\hbar^2 k^2}{2m^*}. \tag{15}$$

Then to calculate the scattering rates in the framework of the quasi-classical approximation it is necessary to do the convolution of W_{Σ}^e and W_{Σ}^a from the space $E \in (-\infty, +\infty)$ to the space $E \in (0, +\infty)$ relative to the final states with zero energy because in the framework of the quasi-classical approximation negative values of the electron kinetic energy are absurd (one can compare, for example, the results of [6] with the results of [17] for the density of final states). So the following equation can be derived

$$\tilde{W}(E) = \Theta(E - \hbar\omega) \left[W_{\Sigma}^e(E) + \Theta(2\hbar\omega - E - E_{\min}) W_{\Sigma}^e(2\hbar\omega - E) \right] + \Theta(E + \hbar\omega) \left[W_{\Sigma}^a(E) + \Theta(-2\hbar\omega - E - E_{\min}) W_{\Sigma}^a(-2\hbar\omega - E) \right]. \tag{16}$$

Here E_{\min} is the minimum energy when the quasi-classical dispersion relation $E = \tilde{\varepsilon}(E) = \int_{-\infty}^{+\infty} S(\varepsilon, E) \varepsilon d\varepsilon$ is still valid in a sufficient accuracy.

The functions of the considered quantities versus the energy E at the temperature $T = 300\text{K}$ are presented in Fig. 3. This figure shows that the discrepancy of the results obtained by means of the different methods is not principal. It proves the evidence of the model presented in this study.

The function $E = E(k)$ calculated by means of Eqs. (5)–(8) under the approximations discussed above is presented in Fig. 4. For comparison, the function $E = E_0(k)$ corresponding to free electrons is shown in this figure, too.

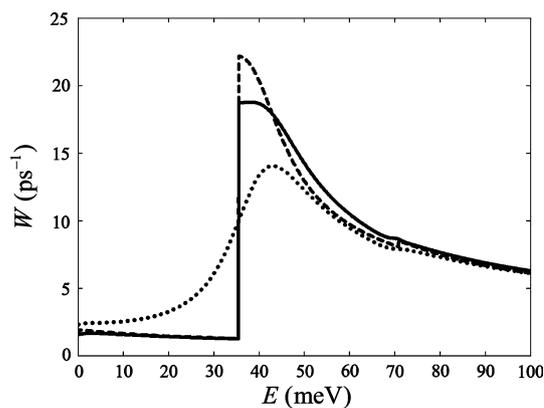


Fig. 3 Polar optical phonon scattering rates in infinitely thin quantum wire. Solid curve: the dependence \tilde{W} on E (Eq. (16)). Dashed curve: the dependence $(W^{e+a} = W^e + W^a)$ on E (Eqs. (10), (11)). Dotted curve: the dependence W_{Σ} on E (Eq. (13))

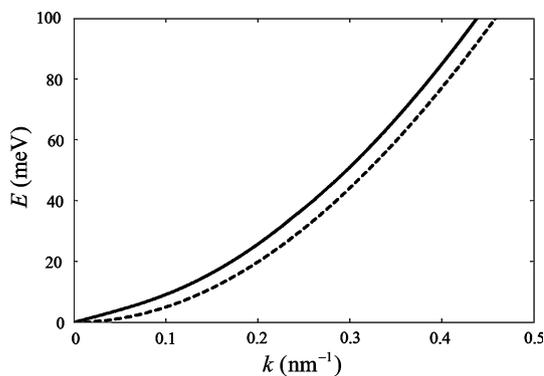


Fig. 4 Energy versus wave vector $E = E(k)$. Solid curve: the dependence calculated by using Eqs. (5)–(8). Dashed curve: the function $E = E_0(k)$

It should be noted that formula (8), in general, can be derived from Eq. (6) accurate to arbitrary constant δE due to the following expression

$$\rho(E) = \left| \frac{dE}{dk} \right|^{-1} = \left| \frac{d(E + \delta E)}{dk} \right|^{-1}. \tag{17}$$

The result presented in Fig. 4 corresponds to $\delta E = 0$.

Calculations of the constant δE are out of the scope of the present study. Nevertheless, it can be assumed that this constant is determined by the following equation

$$\int_0^{\infty} (f_F(E_F, E - \delta E) \rho(E) - f_F(E_F, E) \rho_0(E)) dE = 0. \tag{18}$$

The consequences of this equation are the constant difference between the Fermi energy E_F and the middle of band

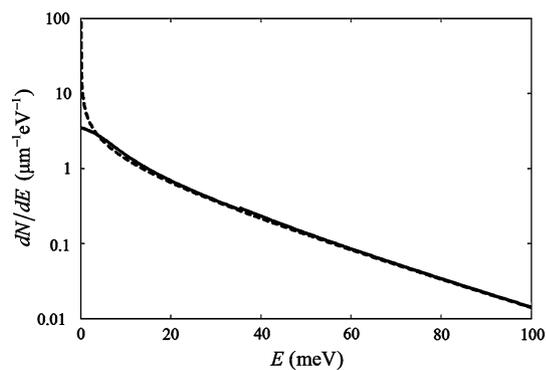


Fig. 5 Function dN/dE versus E . Solid curve: the results calculated by using $\rho(E)$ (Eqs. (5), (6)). Dashed curve: the results calculated by using $\rho_0(E)$

gap as well as conservation of the number of particles in the quantum system. At the same time according to Eq. (18) the difference between the middle of band gap and the ground quantum state energy level calculated by means of the Schrodinger and Poisson equations [5] should decrease at δE , i.e. the shift of the ground quantum state energy level should occur likewise the Lamb shift or the shifts of quasi-stationary energy levels take place in perturbed quantum systems [9, 18]. For the considered case this shift is approximately equal to 5 meV.

Both the function $dN/dE \sim f_F(E)\rho(E)$ taking into account the high-order quantum effects and the function $dN/dE \sim f_F(E)\rho_0(E)$ neglecting them are presented in Fig. 5 (N is the linear concentration of electrons in nanowire). This figure shows that taking into account the high-order quantum effects causes the absence of the discontinuity of the second kind at $E = 0$.

In conclusion, we want to make the note concerning the experimental verification of our theoretical results. The latter can be done using the methods based on interaction of laser radiation with electron gas. So, for example, the qualitative behavior of the dependence presented in Fig. 5 as well as the decrease of the difference between the middle of band gap and the ground quantum state energy level calculated by means of the Schrodinger and Poisson equations can be tested by using the laser pump-probe method [19] conformably to undoped or lightly doped GaAs-in- Al_2O_3 quantum wires.

Thus, in the present study the self-consistent method of calculation of the electron scattering rates in nanowires

with the one-dimensional electron gas in the electric quantum limit is worked out. The developed method allows both the collisional broadening and the quantum correlations between scattering events to be taken into account. Using the approximation of stable one-particle quantum states it is proved that the electron scattering processes determine the dependence of electron energy versus its wave vector.

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References

1. A. Haque, M.R. Quddus, *Solid-State Electron.* **45**, 519 (2001)
2. S.V. Rotkin, K. Hess, *Appl. Phys. Lett.* **84**, 3139 (2004)
3. D.V. Pozdnyakov, V.O. Galenchik, F.F. Komarov, V.M. Borzdov, *Physica E* **33**, 336 (2006)
4. S. Briggs, B.A. Mason, J.P. Leburton, *Phys. Rev. B* **40**, 12001 (1989)
5. A.V. Borzdov, D.V. Pozdnyakov, V.O. Galenchik, V.M. Borzdov, F.F. Komarov, *Phys. Stat. Sol. (b)* **242**, R134 (2005)
6. D.V. Pozdnyakov, V.O. Galenchik, *Phys. Low-Dim. Struct.* **1**, 17 (2006)
7. D.V. Pozdnyakov, V.O. Galenchik, V.M. Borzdov, F.F. Komarov, O.G. Zhevnyak, *Phys. Low-Dim. Struct.* **1**, 19 (2006)
8. D.V. Pozdnyakov, V.O. Galenchik, A.V. Borzdov, *Phys. Low-Dim. Struct.* **2**, 87 (2006)
9. A.S. Davydov, *Quantum Mechanics* (Nauka, Moscow, 1973, in Russian)
10. D. Bohm, *Quantum Theory* (Prentice-Hall, New York, 1952)
11. L.P. Kadanoff, G. Baym, *Quantum Statistical Mechanics. Green's Function Methods in Equilibrium and Nonequilibrium Problems* (W. A. Benjamin, New York, 1962)
12. C. Jacoboni, P. Lugli, *The Monte Carlo Method for Semiconductor Device Simulation* (Springer-Verlag, Wien, New York, 1989)
13. K. Hess (ed.), *Monte Carlo Device Simulation: Full Band and Beyond* (Kluwer Academic Publishers, Boston, Dordrecht, London, 1991)
14. J.M. Ziman, *Electrons and Phonons. The Theory of Transport Phenomena in Solids* (Oxford University Press, Oxford, 2001)
15. M.A. Stroscio, M. Dutta, *Phonons in Nanostructures* (Cambridge University Press, Cambridge, 2001)
16. M.B. Mensky, *Quantum Measurements and Decoherence. Models and Phenomenology* (Kluwer Academic Publishers, Boston, Dordrecht, London, 2000)
17. D.V. Pozdnyakov, V.M. Borzdov, *Phys. Solid State* **45**, 2348 (2003)
18. R.P. Feynman, A.R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill Book Company, New York, 1965)
19. T. Hertel, G. Moos, *Phys. Rev. Lett.* **84**, 5002 (2000)